Accelerated Strategic Computing Initiative

ASCI

at Livermore

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Messina Discusses ASCI's Past Achievements, Future Challenges

Nearing the end of his term as Director of the Office of Advanced Simulation and Computing for Defense Programs in the National Nuclear Security Agency, Paul Messina held an ASCI All-Hands Meeting at the Laboratory in December.

At the beginning of his presentation in the Bldg.132 Auditorium, Messina stated, "I wanted to have the opportunity to tell you in person what a great job you are doing and that the prospects for ASCI are excellent." Concerning the platforms, he noted several indicators of a strong ASCI Program: First, he asserted that "we have three 3-teraOPS systems in place and fully used. ASCI White is in place and will be operational in a few months. Next, the 30-teraOPS machine is on order at Los Alamos. We have the go-ahead to get a system at LLNL that is as close to 100 teraOPS as possible (budget limited) for FY 2004 delivery and to build the Terascale Facility to house it." He added that "Sandia is getting back into the platforms rotation."

Messina also cited additional indicators of ASCI Program health: "We have accomplished all application mileposts on schedule and all ASCI Program elements are contributing, and we have already contributed to directed stockpile work (DSW) and to stockpile stewardship." Messina concluded his list of positive indicators by observing, "Our budget is up again this year."

In listing his predictions for ASCI's future, he stated, "I truly believe that ASCI will stay healthy and be nurtured. Perhaps no big growth, but hey, the ASCI annual budget is approaching $1B. Furthermore, Science-Based Stockpile Stewardship will stay in place. And finally, Congress, DoD, DOE/NNSA, and even other parts of DOE on occasion, all believe that you have been doing a great job.

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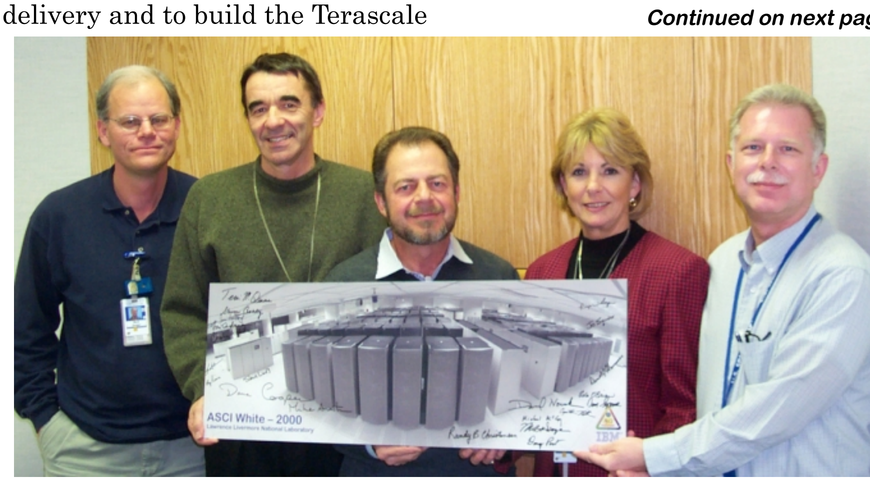


Paul Messina (center) receives an "autographed" poster of ASCI White following his ASCI All-Hands Meeting at LLNL. From the left: Mark Seager, David Nowak, Messina, Rose O'Brien, and Randy Christensen.

Terri Quinn is an Assistant Department Head in SCCD, where she manages the VIEWS Program for ASCI.

Visualizing and Understanding Supercomputing Data

The success of ASCI supercomputers to simulate the physics of nuclear explosions presents a massive data challenge: making sense of the enormous amounts of data generated by the supercomputers and the advanced computer codes. ASCI's Data Assessment Theater is one approach being used. This facility became operational in December 1998, representing one of the highest resolution scientific display capabilities in the country. This precedent-setting facility represents the highest-end user interface for data analysis and manipulation. It utilizes 15 state-of-the-art projectors to achieve 6,400 × 3,072 pixel resolution and superior image quality on an 8- × 16-ft screen. Driving these projectors as well as driving displays in weapon scientists' offices are two large SGI computers with a total of 104 300-MHz processors, 26 Infinite Reality (IR) graphics pipes, and 20 terabytes of fast disk. The aggregate I/O rate to these servers is over 1.5 gigabytes/sec.

Continued on page 4

"You have proven many skeptical people wrong," Messina continued. "You have gotten huge computers up and made them usable. You reinvigorated high-end scientific computing worldwide and met a number of those pesky mileposts, which are helping to build the needed capabilities. You have built world-class visualization facilities, devised and implemented algorithms that have helped ASCI codes meet their mileposts. At LANL, the Strategic Computing Center is well underway towards completion on schedule and on budget. We have contracts in place for our high-bandwidth Tri-Lab network, soon to be deployed. In addition, we have developed software that others want (system software, applications, etc.). We inspired some top notch universities to become much more active in CS&E (including new courses, degree programs) and in multidisciplinary computing projects. With all those accomplishments and more, it is no wonder that ASCI has earned respect and support from so many people."

Messina concluded his remarks by reminding his audience about the importance of our taking a "system view"—the integration of nearly all elements of ASCI into new, unprecedented simulation capabilities. "Few, if any, programs get to tackle essentially all aspects of technical computing, end-to-end, and with adequate resources. Agreement on de facto standards is important and will pay off. Stay connected to the rest of Defense Program activities, especially DSW and experimental facilities, and keep in touch with the rest of the scientific computing community."


Doug Post (left) and Paul Messina share stories at the luncheon following Messina's ASCI All Hands Meeting. Post is headed for Los Alamos and Messina is returning to Caltech.

Messina's talk was followed by a question and answer session, then a luncheon where he was presented with a poster of ASCI White, signed by many of his LLNL colleagues.

While in Defense Programs, Paul Messina worked to get Tri-Lab support for ASCI principles and goals through 2010 and agreement on the appropriate associated budget. He worked to form partnerships with industry, academia, and other government laboratories to tap into appropriate technology and talent. He was acknowledged for leading a new, startup program and bringing stability, credibility, and respectability to it.

Paul Messina plans to take a vacation and return to the California Institute of Technology (Caltech) from which he took a two-year leave of absence. At Caltech, he is Assistant Vice President for Scientific Computing, Faculty Associate in Scientific Computing Research, and Director of Caltech's Center for Advanced Computing Research. He also took leave from the position of Chief Architect for the National Partnership for Advanced Computational Infrastructure, established by NSF and led by the University of California, San Diego.

Doug Post Heads for Los Alamos

Doug Post, the Associate Division Leader for Computational Physics for A-Division and the Group Leader for ICF Code Development in X-Division at LLNL since 1998, has accepted a new position at Los Alamos. In early February, Doug will become the Deputy Division Director for Computational Methods and Simulation, Applied Physics (X) Division at LANL. He will be responsible for computational physics for X Division, which is the Los Alamos equivalent of A, B, and X Divisions at LLNL. His new job at LANL is roughly the sum of his present A-Division position and the equivalent B Division position, plus the additional responsibility for V&V, turbulence, and materials modeling for X Division.

From 1968 to 1971, Doug was a designer and code developer in B Division at the Lab. He was a device physicist on the MINT LEAF test with Bill Scanlin. He also did ICF design studies with Jim Wilson. He wrote the first multi-group flux-limited transport code with Jim Wilson and Jim LeBlanc.

In 1971, he returned to graduate school at Stanford. Upon graduation, he went to Princeton and established a group to model tokamaks. He applied modeling tools to analyze and predict the performance of tokamak experiments, and to aid in the design of "next-step" tokamaks. From 1988–1990, he led the International Thermonuclear Experimental Reactor (ITER) Physics Project, coordinating the efforts of the 200 physicists in Europe, Japan, Russia, and the US supporting the ITER. When the US dropped out of ITER in 1998, Doug returned to the Lab where he was the Associate Division Leader for Computational Physics in A-Division. Since March 16, 1998, he has coordinated the code development programs in A and X Division. Doug feels that "the major accomplishments of the A-Division code projects have been to successfully provide and support modern production codes for the directed stockpile work (DSW) and campaign designers while simultaneously developing new ASCI codes with the improved physics and resolution needed for the future."

"Doug's leadership, savvy insight, and commitment to the ASCI goals will be sorely missed at LLNL," noted ASCI Program Leader David Nowak. "We wish him well and extend our gratitude for his many contributions."

May's Book Examines "Parallel I/O from the Bottom Up"

John May, a group leader for Computer Science in the Center for Applied Scientific Computing (CASC), recently published a book entitled *Parallel I/O for High Performance Computing* (366 pp., Morgan Kaufmann Publishers, ISBN-1558606645).

Parallel I/O for High Performance Computing provides an overview of key I/O issues at all levels of abstraction—including hardware, through the OS and file systems, up to very high-level scientific libraries. May describes the important features of MPI-IO, netCDF, and HDF-5 and presents numerous examples illustrating how to use each of these I/O interfaces. In addition, he addresses the basic question of how to read and write data efficiently in HPC applications. Further, he discusses various layers of storage and techniques for using disks (and sometimes tapes) effectively in HPC applications.

May maintains that scientific and technical programmers can no longer afford to treat I/O as an afterthought. The speed, memory size, and disk capacity of parallel computers continue to grow rapidly, but the rate at which disk drives can read and write data is improving far less quickly. Consequently, the performance of carefully tuned parallel programs can slow dramatically when they read or write files. May contends that the problem is likely to get far worse.

John May's book "Parallel I/O for High Performance Computing" discusses high-performance I/O in a data-centric world.

Parallel input and output techniques can help solve this problem by creating multiple data paths between memory and disks. However, simply adding disk drives to an I/O system without considering the overall software design will not significantly improve performance. To reap the full benefits of a parallel I/O system, application programmers must understand how parallel I/O systems work and where the performance pitfalls lie.

Parallel I/O for High Performance Computing directly addresses this critical need by examining parallel I/O from the bottom up. Alan Sussman at the University of Maryland notes, "This text provides a useful overview of an area that is currently not addressed in any book. The presentation of parallel I/O issues across all levels of abstraction is this book's greatest strength."

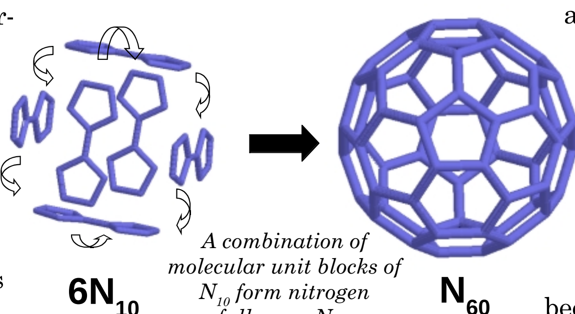
John May joined LLNL in 1994 after receiving his Ph.D. in Computer Science from the University of California, San Diego. His interests include parallel programming models, performance analysis, parallel I/O, and parallel programming tools.

May's publishing effort received some funding support from the ASCI Institute for Terascale Simulation (ITS), which sponsors in-house research and collaborative research with academia in areas of computer science, computational mathematics, and scientific computing relevant to the Stockpile Stewardship Program. *Parallel I/O for High Performance Computing* may be ordered from local bookstores or through most online booksellers.

Nitrogen Bucky Ball

The possible existence of polymeric forms of nitrogen, in which the strong triple bond of the diatom is transformed and replaced by single or single and double bonds, is of a particular interest because of the energetic properties associated with these materials. As potential high-energy density materials from an abundant natural source, they become leading candidates for alternative energy storage media. This has led to extensive research on such exotic species as tetrahedral N_4 and cubic N_8.

In a recent computational study, Riad Manaa, a theoretical chemist who conducts research on the properties of energetic materials in the ASCI Program, suggested that a super-high energy molecule N_{60} could be formed from six units of bicyclic N_{10} molecules, as shown in the figure. The molecule is analogous to the famous soccer-ball-shaped C_{60}, which ignited dramatic advances in fullerene and nanotubes science since its discovery in the mid 1980s.



A combination of molecular unit blocks of N_{10} form nitrogen fullerene, N_{60}.

Manaa used quantum mechanical-based electronic structure techniques to study the structure of N_{10}. His results showed that N_{10} contains a mixture of single and double bonds and could be relatively stable. He then proposed that six N_{10} molecules might be able to form a buckminster molecule of N_{60} under extreme conditions of pressure. Manaa is currently conducting simulations to determine the stability of N_{60} and analogous boron-based molecular species. Manaa notes, "The use of extensive and rigorous computational tools coupled with the relatively large size of these molecules renders the use of massively parallel platforms—such as ASCI Blue—of paramount necessity."

Riad Manaa's research has been published in *Chemical Physics Letters*, **331**, 262 (2000) and has attracted attention from the media: *Chemical & Engineering News* (the weekly magazine of the American Chemical Society) on December 18; *NewsLine*'s December 22 issue; and the *Tri Valley Herald* on January 4.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

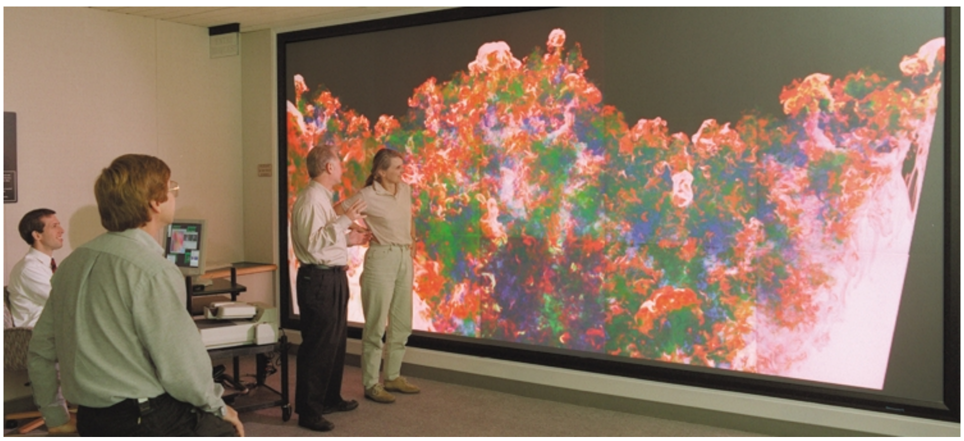
Large facilities like our Data Assessment Theater are designed for small teams of scientists to evaluate and present simulation data quickly. Perhaps more importantly are the capabilities in the scientists' offices because much of the work in evaluating simulation data takes place in individual offices. To this end, we are deploying fast video connections and high-density displays in scientists' offices—connecting to the same computer resources used by the Data Assessment Theater. While only a few weapon scientists now enjoy this capability, we will triple that number soon. To provide this support to more weapon scientists, and indeed to other scientists at the lab, demands a breakthrough to reduce the cost. We are working with Stanford University, Los Alamos, and Sandia to accomplish this and perhaps to revolutionize scientific visualization—a topic for a future *ASCI at Livermore* newsletter.

The rapid advance of the ASCI computer platforms mandates a comparable rapid advance in software. A parallel runtime system and a parallel software development environment are two software components needed to enable parallel simulations. The run-time system is the software middleware that allows applications to use the cluster of hardware as a single system, enabling parallelism on ASCI platforms. The software development environment allows ASCI simulation developers to write parallel codes to run on these unique systems.

In FY99, we established a PathForward project, Ultrascale Tools, to advance the parallel software development environment.

In FY00, we added a new PathForward project to accelerate runtime system technologies. These combined efforts total $14M for software R&D and encompass four years and four companies—thus accelerating needed high-performance software technologies.

—Terri Quinn



ASCI's Data Assessment Theater. Driven by a multi-processor visualization server, interactive applications can be displayed at very high resolution on this 15-projector display wall. From the left, Sean Ahern, Ross Gaunt, Randy Christensen, and Terri Quinn.

Editor Whitney Lacy Joins CASC Team

Whitney Lacy is the new editor at CASC.

Whitney Lacy is the new technical editor/writer supporting the Center for Applied Scientific Computing (CASC). Whitney comes to the Lab from Economic & Planning Systems, Inc., a Berkeley-based land use economics consulting firm, where she edited reports, proposals, and brochures. Previously, Whitney worked at Freedom from Hunger in Davis, California, also as an editor. Whitney is orginally from Arizona and has travelled extensively in Europe and Australia. She has a Bachelor of Fine Arts degree from the University of Arizona. Whitney's office is Rm. 2007 in Bldg. 451, and her email address is wlacy@llnl.gov.

ASCI at Livermore is published by the Accelerated Strategic Computing Initiative Program, a division of the Defense and Nuclear Technologies Directorate at Lawrence Livermore National Laboratory. Please send corrections and contributions to Tim Peck, (925) 424-6251 and peck7@llnl.gov.